Secrets of a New Superconductor, Magnesium Diboride, Revealed

A team of theorists lead by Marvin Cohen and Steven Louie have calculated the properties of magnesim diboride (MgB_2) from first principles and, in doing so, have explained the origin of its unexpected superconducting behavior.

In January 2001, a research group in Japan headed by Akimitsu discovered that MgB_2 becomes superconducting at 39 Kelvin, giving it one of the highest known transition temperatures (T_c) of any superconductor. Hundreds of papers have been produced in the first rush to examine this material, but experimenters using different techniques have reported many different, often unusual, and sometimes conflicting properties. For example, there was some evidence that MgB_2 might have more than one superconducting "energy gap," a property that had been anticipated in theory but had never before been seen experimentally. Further, MgB_2 is a layered material like the cuprate ceramic high-T_c superconductors, but while undoped cuprates are insulators at ordinary temperatures, it was observed that MgB_2 is always a metallic conductor. With the publication of these and other results, it quickly became apparent that theories developed to explain superconductivity in the high-T_c cuprates would not be helpful in understanding MgB_2.

Louie and Cohen and their colleagues used the well-established Bardeen-Cooper-Schrieffer (BCS) theory that had been developed for low T_c superconductors to examine the fundamental properties of MgB_2. In order to do this, the group developed a new technique to solve the BCS equations for materials with complex electronic structure. The calculations were performed at the Department of Energy's National Energy Research Scientific Computing Center (NERSC).

In BCS theory, electrons overcome their mutual repulsion to form pairs that can move through the material without resistance. Vital to pair formation are the quantized vibrations of the crystal lattice, known as phonons. What was puzzling was that according to the simplest form of BCS theory, the interaction between the lattice and the electrons, which is required to form an electron pair, should be equivalent to the interaction between the lattice and a single electron emitting and reabsorbing a phonon itself. But in MgB_2 these two values were apparently different—a clue that more than one kind of electron might be involved in pairing. In fact there are two separate populations of electrons—nicknamed "blue" and "gold"—that form different kinds of bonds with the material's atoms. The two kinds of electrons are coupled, and as the temperature is increased, the superconducting gaps (i.e., the energy required to place a single electron into a "blue" or "gold" state) rapidly converge to zero, until at about 39 K both vanish. Above this temperature, all pairs are broken and the material does not superconduct. The theoretical confirmation that there indeed is more than one superconducting "energy gap" in these materials and the calculation of the temperature dependence of the behavior of the "blue" and "gold" electrons made it possible to interpret the full spectrum of the experimental measurements, including those from scanning tunneling microscopy, optical studies, electron photoemission, and neutron analyses, and from heat capacity and infrared studies.

BCS theory contemplated the possible existence of materials with multiple superconducting energy gaps early on; in this context, this new understanding of MgB_2 offers a new model for the discovery of materials capable of high-temperature superconductivity. Such work is in progress.

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Hyoung Joon Choi, David Roundy, Hong Sun, Marvin L. Cohen, and Steven G. Louie, "The origin of the anomalous superconducting properties of MgB2," *Nature* **418**, 758 (2002).